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(FILE 'HOME' ENTERED AT 08:03:26 ON 15 JUN 2004)

FILE 'CA' ENTERED AT 08:03:55 ON 15 JUN 2004

L1 142067 S CATALY?(5A) (ANALY? OR ASSAY? OR ASSES? OR CHARACTERIZ? OR  
DETECT? OR DETERMIN? OR DISCOVER? OR ESTIMAT? OR EVALUAT? OR  
EXAMIN? OR EXPLOR? OR IDENTIF? OR INVESTIGAT? OR MEASUR? OR  
MONITOR? OR PROBE# OR PROBING OR SCREEN? OR SENSE# OR SENSING OR  
SENSOR OR STABIL? OR STUDY? OR STUDIE#)  
L2 19669 S CATALY?(5A) (POISON? OR QUANTITAT? OR QUANTIF? OR TEST?)  
L3 1520 S L1-2(10A) (PARALLEL OR SIMULTAN? OR COMPLET? OR FULL?)  
L4 2259 S L1-2 AND MASS SPECTRO?  
L5 2004 S L1-2 AND(THERMOCOUPLE? OR TEMPERATURE(3A) (SENSOR OR SENSING OR  
SENSE# OR DETECT? OR MEASUR? OR MONITOR? OR PROBE#))  
L6 36 S L4 AND L5  
L7 239 S L3 AND (REACTOR OR MINIREACTOR OR MICROREACTOR)  
L8 55 S L3 AND L4-5  
L9 92 S L3 AND(INFRARED OR INFRA RED OR NIR OR FTIR)  
L10 392 S L6-9  
L11 289 S (L10 NOT PY>2000) OR (L10 AND PATENT/DT AND PY<2002)  
L12 1167 S L1-2 (10A) (COMBINE# OR COMBINATION OR COMBINING) NOT L3  
L13 1357 S L1-2 (10A) (TWO OR THREE OR FOUR OR MULTIPLE OR DIFFERENT OR  
PLURAL?) (5A) (DETECT? OR DETERMIN? OR MONITOR? OR MEASUR? OR  
SPECTRO? OR SENSOR) NOT L3  
L14 303 S L12 AND(L4-5 OR INFRARED OR INFRA RED OR NIR OR FTIR OR REACTOR  
OR MINIREACTOR OR MICROREACTOR)  
L15 229 S (L14 NOT PY>2000) OR (L14 AND PATENT/DT AND PY<2002)  
L16 506 S L11,L15 NOT(FULL LOAD OR KRAFT OR TURBINE OR SHIPBOARD OR  
PARTIAL WETTING OR IRIIDIUM ELECTRODE)  
L17 481 S L16 NOT(TOKAMAK OR NUCLEAR REACTOR OR PROTEIN OR PROTIEEN OR  
ENZYM? OR INSECTICIDE OR CLEAN GAS OR FUEL CELL)  
L18 471 S L17 NOT(PHOTOLYSIS OR BIOTIN OR STRATOS? OR SCALEUP OR ISOTOP?  
EFFECT?)

=> d bib,ab 1-471 118 y

L18 ANSWER 3 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 135:319840 CA  
TI Parallel **reactor** with internal sensing  
IN Turner, Howard W.; Dales, G. Cameron; Vanerden, Lynn; Van Beek,  
Johannes A. M.  
PA Symyx Technologies, USA  
SO U.S., 57 pp., Cont.-in-part of U.S. Ser. No. 177,170.  
PI US 6306658 B1 20011023 US 1998-211982 19981214 <--  
US 6548026 B1 20030415 US 1998-177170 19981022  
PRAI US 1998-96603P P 19980813  
AB An app. and method for carrying out and monitoring the progress and  
properties of multiple reactions is disclosed. The method and app. are  
esp. useful for synthesizing, screening, and characterizing  
combinatorial libraries, but also offer significant advantages over  
conventional exptl. **reactors** as well. The app. generally includes

multiple vessels for contg. reaction mixts., and systems for controlling the stirring rate and temp. of individual reaction mixts. or groups of reaction mixts. In addn., the app. may include provisions for independently controlling pressure in each vessel, and a system for injecting liqs. into the vessels at a pressure different than ambient pressure. In situ monitoring of individual reaction mixts. provides feedback for process controllers, and also provides data for detg. reaction rates, product yields, and various properties of the reaction products, including viscosity and mol. wt.

L18 ANSWER 4 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 135:309410 CA

TI Catalyst characterization apparatus

IN Moon, Dong Ju; Park, Kun You; Chung, Moon Jo; Ahn, Byoung Sung

PA Korea Institute of Science and Technology, S. Korea

SO U.S., 10 pp., Cont. of U.S. Ser. No. 45,175, abandoned.

PI US 6306349 B1 20011023 US 1999-449467 19991129 <--

PRAI KR 1997-9808 A 19970321

AB The present invention relates to a catalyst characterization app., and in particular to an improved catalyst characterization app. which is capable of characterizing the surface of a catalyst more accurately by a volumetric method without requiring a pre-treatment step which may vary the characteristics of the catalyst as well as without exposing the catalyst in air, by combining a dynamic flow type **reactor** with a volumetric type adsorption app., whereby it is possible to accurately characterize the catalyst during an actual reaction. It is possible to accurately characterize the various **catalysts** and to **characterize** the **catalyst** during the reaction, alternately and/or continuously, by **combining** a dynamic flow type **reactor** with a volumetric type characterization app. as well as a dynamic flow type characterization app.

L18 ANSWER 6 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 135:51670 CA

TI Process for **simultaneously evaluating** a plurality of **catalysts**

IN Akporiaye, Duncan E.; Karlsson, Arne; Dahl, Ivar M.; Wendelbo, Rune; Vanden Bussche, Kurt M.; Towler, Gavin P.

PA UOP LLC, USA

SO PCT Int. Appl., 20 pp.

PI WO 2001044801 A2 20010621 WO 2000-US32422 20001214 <--

US 6627445 B1 20030930 US 1999-464313 19991215

PRAI US 1999-464313 A 19991215

AB A process for **simultaneously testing** a plurality of **catalysts** using combinatorial chem. has been developed. The process involves contg. the plurality of catalysts in an array of parallel **reactor** contg. a bed of catalyst. Each bed of catalyst is then simultaneously contacted, at reaction conditions, with a reactant to form an effluent of each **reactor**. The reactant or an inert fluid is at a space velocity sufficient to fluidize the catalyst beds. Each of the effluents is analyzed.

L18 ANSWER 13 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 134:210416 CA

TI Automated method and apparatus for **simultaneous evaluation** of multiple **catalysts** in multiple **reactors**

IN Deves, Jean Marie; Bernhard, Jean Yves; Chatelain, Bernard; Toutant, Pierre; Brandely, Jose; Guitton, Corinne

PA Institut Francais du Petrole, Fr.

SO Fr. Demande, 28 pp.

PI FR 2795513 A1 20001229 FR 1999-8282 19990628 <--

US 6551832 B1 20030422 US 2000-604731 20000628

PRAI FR 1999-8282 A 19990628

AB A method and app. was described for carrying out measurements on the product of a chem. reaction in the presence of a **catalyst**, esp. for **simultaneous evaluation** of multiple **catalysts** in a **reactor** array. The method and app. are characterized by: (1) at least two **reactors**, (2) means for sepn. of gas and liq. phases downstream of each **reactor**, (3) distribution means for controlled transfer of the gas phase from the phase sepn. device to the first anal. chamber, (4) a second anal. chamber for measuring the liq. phase from the phase sepn. device, and (5) a means for automatic control of the chem. reaction parameters, for transferring product streams, and for anal. of the sepd. gas and liq. phases. The method is esp. useful for evaluation of petroleum refining catalysts.

L18 ANSWER 19 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 133:363946 CA

TI In Situ Investigations of Structural Changes in Cu/ZnO Catalysts

AU Grunwaldt, J.-D.; Molenbroek, A. M.; Topsoe, N.-Y.; Topsoe, H.; Clausen, B. S.

CS Haldor Topsoe Research Laboratories, Lyngby, DK-2800, Den.

SO Journal of Catalysis (2000), 194(2), 452-460

AB Dynamic changes in the structure and catalytic activity of Cu/ZnO methanol synthesis **catalysts** were **studied** by an in situ method, which **combines** x-ray diffraction, x-ray absorption fine structure spectroscopy (XAFS), and online **catalytic measurements** by **mass spectrometry**. The temp.-programmed redn. of copper was monitored by in situ quick-EXAFS (QEXAFS) and online **mass spectrometry**. Under typical mild redn. conditions, small copper particles (10-15 Å) are formed. Upon change in the redn. potential of methanol synthesis gas, reversible changes of the Cu-Cu coordination no. are obsd. by EXAFS. These structural changes are accompanied by changes in the catalytic activity and the highest activity was obsd. after exposure to the most reducing conditions. In this state the catalyst exhibited low Cu-Cu coordination nos. These results support the model that reversible changes in the wetting of ZnO by Cu may occur upon changes in the reaction conditions and that such dynamic changes in Cu morphol. may influence the catalytic properties. The conditions used in the studies are less severe than those that result in bulk alloy formation. However, addnl. XAFS **measurements** at higher **temps.** were performed and EXAFS spectra were simulated to address the possibility for Cu-Zn alloy formation as suggested by recent results in literature. Only under

severe redn. conditions was significant alloying of copper and zinc obsd. in EXAFS in addn. to the morphol. changes. Such changes have not been seen in the Cu/SiO<sub>2</sub> system.

L18 ANSWER 23 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 133:270709 CA

TI In situ FT-IR study of the selective catalytic reduction of NO by propane on Cu-ZSM-5: evidence of a reaction pathway by oxygen pulses  
AU Poignant, F.; Freysz, J. L.; Daturi, M.; Saussey, J.; Lavalley, J. C.  
CS Laboratoire de Catalyse et Spectrochimie, Caen, 14050, Fr.

SO Studies in Surface Science and Catalysis (2000), 130B(International Congress on Catalysis, 2000, Pt. B), 1487-1492

AB SCR of NO by propane has been **investigated** on Cu-ZSM-5 **catalyst** using in situ FT-IR spectroscopy in a **reactor** cell **combined** with online MS and IR gas anal. We have operated in transient conditions, adding oxygen pulses in a propane + NO flow to put in evidence the reactivity of surface intermediates. A reaction pathway has been derived, which involves the formation and evolution of isocyanide and isocyanate intermediates, as well as adsorbed ammonia, coordinated with Cu<sup>+</sup>.

L18 ANSWER 41 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 132:353245 CA

TI **Simultaneous screening of catalysts** in microchannels: Methodology and experimental setup

AU Zech, Torsten; Honicke, Dieter; Lohf, Astrid; Golbig, Klaus; Richter, Thomas

CS Lehrstuhl für Technische Chemie, Technische Universität Chemnitz, Chemnitz, D-09107, Germany

SO Microreaction Technology: Industrial Prospects, Proceedings of the International Conference on Microreaction Technology, 3rd, Frankfurt, Apr. 18-21, 1999 (1999), 260-266. Editor(s): Ehrfeld, Wolfgang. Publisher: Springer-Verlag, Berlin, Germany.

AB Given the excellent properties of microfluidic **reactors** our project aims to develop a fast and parallelized **catalyst screening** unit. In a first step the channel-walls of microstructured wafers are coated with catalytic active species. For the **screening of catalytic** properties a stack of 35 catalyst wafers is operated under steady-state conditions and continuous flow. Each wafer is exposed to the same amt. of reactant gases at the same time, temp. and pressure. The product anal. is carried out using **mass spectrometry** for each catalyst wafer in order to gain full chem. information of the product distribution, conversion degrees and selectivities. A fast, sequentially sampling device is used to sample each catalyst wafer at least every 60 min.

L18 ANSWER 45 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 132:226551 CA

TI Behavior of Palladium-Copper Catalysts for CO and NO Elimination

AU Fernandez-Garcia, M.; Martinez-Arias, A.; Belver, C.; Anderson, J. A.; Conesa, J. C.; Soria, J.

CS Instituto de Catalisis, CSIC, Campus Cantoblanco, Madrid, 28049, Spain  
SO Journal of Catalysis (2000), 190(2), 387-395

AB The behavior of a series of Pd and Pd-Cu catalysts supported by CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> for the CO+NO+O<sub>2</sub> reaction was analyzed by a **combination** of electron transmission microscopy, **IR**, and electron paramagnetic spectroscopies and **catalytic test studies**. In both systems, catalytic behavior was dominated by the properties of the metal-CeO<sub>2</sub> interface. Adding Cu to a Pd system led to beneficial effects related to alloy formation in which both CO and NO elimination were enhanced. The chem. consequences and catalytic implications of Pd-Cu alloying are discussed.

L18 ANSWER 59 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 132:12044 CA

TI High-throughput **testing** of heterogeneous **catalyst** libraries using array **microreactors** and **mass spectrometry**

AU Senkan, Selim; Krantz, Kevin; Ozturk, Sukru; Zengin, Veysel; Onal, Isik  
CS Department of Chemical Engineering, University of California, Los Angeles, CA, 90095, USA

SO Angewandte Chemie, International Edition (1999), 38(18), 2794-2799

AB In the array described here, four **microreactors**, each having 20 channels, were stacked and placed inside an aluminum heating block. The results of time-onstream testing of a platinum/palladium/indium library with 66 combinations for the catalytic dehydrogenation of cyclohexane to benzene were reported. Thus it was possible to **test** 80 different **catalysts** in **parallel**.

L18 ANSWER 64 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 131:313588 CA

TI Influence of Ceria on Pd Activity for the CO+O<sub>2</sub> Reaction

AU Fernandez-Garcia, M.; Martinez-Arias, A.; Salamanca, L. N.; Coronado, J. M.; Anderson, J. A.; Conesa, J. C.; Soria, J.

CS Instituto de Catalisis y Petroleoquimica, CSIC, Campus Cantoblanco, Madrid, 28049, Spain

SO Journal of Catalysis (1999), 187(2), 474-485

AB The behavior of a series of palladium catalysts supported on alumina, ceria, and ceria/alumina for the CO + O<sub>2</sub> reaction has been analyzed by a **combination** of electron transmission microscopy, **IR**, and ESR spectroscopies and **catalytic test studies**. Ceria is shown to decrease the onset of the reaction by ~130 K due to an enhanced activation of both reactant mols. Even at room temp., ceria facilitates activation of CO by promoting the formation of metallic palladium and that of oxygen by the presence of reactive vacancies at the Pd-Ce interface. The optimum ceria-promoting effect in the CO conversion is obsd. for palladium particles in contact with 3-dimensional ceria supported particles, which seem to be oriented by their interaction with alumina, and is ascribed to the specific characteristics of the anionic vacancies located at the corresponding Pd-Ce interface. The bulk ceria support, however, induces an oxidn.-deactivation of palladium at medium and high reaction temps. which hinders reaction between Pd-bonded CO and Ce-bonded oxygen at the Pd-Ce interface.

L18 ANSWER 71 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 131:222760 CA

TI In-line **catalytic** derivatization method for selective **detection** of chlorinated aromatics with a hyphenated gas chromatography/laser **mass spectrometry** technique: a concept for comprehensive detection of isomeric ensembles

AU Zimmermann, Ralf; Rohwer, Egmont R.; Heger, Hans Joerg

CS Institut fuer Oekologische Chemie, GSF-Forschungszentrum fuer Umwelt und Gesundheit, Oberschleissheim, D-85764, Germany

SO Analytical Chemistry (1999), 71(19), 4148-4153

AB The combination of gas chromatog. (GC) and laser-based resonance-enhanced multiphoton ionization-time-of-flight **mass spectrometry** (REMPI-TOFMS) represents a three-dimensional anal. method, using the gas chromatog. retention time, the wavelength of the ionization laser for REMPI, and the mol. mass as anal. parameters. A novel anal. scheme for detection of chlorinated arom. compds., including isomeric ensembles, by GC/REMPI-TOFMS is presented. The concept uses an in-line hydrodechlorination catalyst for post- or precolumn derivatization of chlorinated arom. compds. The chlorinated aroms. are quant. reduced, forming their resp. arom. skeletons. These arom. skeletons are detected selectively by REMPI-TOFMS. The 1st results for substance class selective detection of chlorinated benzene isomers are given, and potential applications in the field of the anal. of compds. such as polychlorinated dibenzo-p-dioxins and -furans are discussed.

L18 ANSWER 73 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 131:201770 CA

TI Microwave induced chemical reactions in synthesis and catalysis

AU Suib, Steven L.; Vilenko, Elizabeth; Zhang, Qihua; Marun, Carolina; Conde, L. Daniel

CS U-60, Department of Chemistry, University of Connecticut, Storrs, CT, 06269-4060, USA

SO Ceramic Transactions (1997), 80(Microwaves: Theory and Application in Materials Processing IV), 331-339

AB The use is studied of microwave heating in the presence and absence of catalysts for conversion of methane into higher hydrocarbons via oligomerization reactions. In addn., microwave-induced heating of precursors of manganese oxide sols and gels have been used to prep. highly dispersed microporous manganese oxides used as oligomerization catalysts. Optimization of reactor types, modes of operation (contact times, pulse vs. continuous), and addn. of dielects. are used to optimize conversion and selectivity. In-situ characterization methods are developed to monitor the mechanisms of reaction. The goals of this research are to prep. microporous MnO<sub>2</sub> microwave-induced oligomerization (MIO) **catalysts**, to **study** MIO of methane to higher hydrocarbons, to elucidate mechanistic details of MIO reactions, and to study fundamental aspects of reactor configuration, additives (chain propagators, dielects.), **temp. measurements**, magnetic field effects, and reaction conditions. All reactions are carried out in a flow system. Characterization studies have involved product analyses by gas chromatog. **mass spectrometry** methods, and Fourier transform IR studies of hydrocarbon intermediates and products. Such studies are believed

to involve absorption of microwaves by a catalyst followed by energy transfer to reactant mols. at the solid-gas interface.

L18 ANSWER 87 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 130:326976 CA

TI A technique for **simultaneous** in-situ MAS NMR and online gas chromatographic **studies** of hydrocarbon conversions on solid **catalysts** under flow conditions

AU Hunger, Michael; Seiler, Michael; Horvath, Thomas

CS Institute of Chemical Technology I, University of Stuttgart, Stuttgart, D-70550, Germany

SO Catalysis Letters (1999), 57(4), 199-204

AB A new technique was introduced for simultaneous in-situ MAS NMR investigations of hydrocarbon conversions on solids under flow conditions and online gas chromatog. For adsorption of MeOH on zeolite H-Beta, equal amts. of adsorbed mols. were detd. by both anal. methods. Studying the synthesis of Me tert-Bu ether (MTBE) on zeolite H-Beta using an MAS NMR rotor **reactor**, a const. yield of MTBE of 27% was obtained up to a wt. hourly space velocity of 1.4 h<sup>-1</sup>. The variation of the reaction temp. led to a simultaneous change of the <sup>13</sup>C MAS NMR signals of isobutoxy species and of the yield of MTBE detd. by online gas chromatog., which indicated that isobutoxy species act as the chem. active compds. In this first application, the new in-situ technique has demonstrated its advantage for a simultaneous investigation of compds. with a long residence time on the catalyst surface and of compds. rapidly leaving the catalyst surface.

L18 ANSWER 88 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 130:317077 CA

TI Discovery and optimization of heterogeneous catalysts by using combinatorial chemistry

AU Senkan, Selim M.; Ozturk, Sukru

CS Los Angeles Department of Chemical Engineering, University of California, Los Angeles, CA, 90095-1592, USA

SO Angewandte Chemie, International Edition (1999), 38(6), 791-795

AB We report herein on the application of REMPI together with novel array **microreactors** for the discovery of an optimal compn. in the ternary Pt/Pd/In metal catalyst system for the dehydrogenation of cyclohexane to benzene. Array **microreactors** allow the **screening** of a large no. of **catalysts** in **parallel** and under identical (std.) operating conditions. Consequently, measurements become primarily sensitive to the method of prepn. of the catalysts. This represents a significant advance over the current practice in catalyst research, in which different catalysts are often studied under different operating conditions, rendering comparisons difficult.

L18 ANSWER 98 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 130:5434 CA

TI How transient kinetics may unravel methane activation mechanisms

AU Mirodatos, C.

CS Institut de Recherches sur la Catalyse, Villeurbanne, Fr.

SO Studies in Surface Science and Catalysis (1998), 119(Natural Gas Conversion V), 99-106

AB A review with 33 refs. Novel routes for direct conversion of methane into higher hydrocarbons and oxygenates were investigated during the last decades, in parallel with a renewed interest for the indirect routes through syngas formation. For the latter, despite a large research effort on a less heat-consuming process such as partial oxidn., engineering problems (heat and mass transfer control) have still to be solved and catalysts to be improved. For this, a precise knowledge of the related mechanisms and microkinetics is required. In a study confined to the steady-state kinetics, only lumped kinetic parameters can be estd. from a regression of steady-state kinetic data. By generating transients input signals, one observes signals out of the steady-state, the relaxation of which may be related to the time scale on which the corresponding global reaction occurs at the steady-state. The steady-state isotopic transient kinetic anal. consists in generating isotopic step functions which let the overall surface occupancy unperturbed and therefore gives access to true time consts. of the reactive intermediates and to their concn. It can also be combined with in situ diffuse reflectance IR spectroscopy (DRIFT). In the temporal anal. of product (TAP) **reactor** transient kinetics are generated by pulsing small and known amts. of reactants through a catalyst bed maintained under vacuum and analyzing the pulse expansion and relaxation at the **reactor** exit with a time resolu. below the millisecond. Recent reviews demonstrate the unique power of these techniques to **investigate catalytic** phenomena (non uniform surface, **combination** of kinetic, thermal and hydrodynamic parameters. This paper aims at illustrating some recent application of these techniques for unraveling the complex mechanisms of methane reforming and methanation.

L18 ANSWER 113 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 129:54054 CA

TI A **combined** approach to **characterization** of **catalytic** reactions using in situ kinetic **probes**

AU LeBlond, C.; Wang, J.; Larsen, R.; Orella, C.; Sun, Y.-K.

CS Merck Research Laboratories, Merck & Co., Inc., Rahway, NJ, 07065, USA

SO Topics in Catalysis (1998), 5(1-4, Fine Chemicals Catalysis, Pt. 2), 149-158

AB Several in situ probes for continuously monitoring rate of catalytic reactions under reaction conditions are described. They are reaction calorimetry, measurements of hydrogen uptake in the case of hydrogenation, and IR spectroscopy. In studying catalytic hydrogenation reactions, for example, these in situ probes provide kinetic details of the reactions from different perspectives over the entire course of the reaction. The reaction calorimetry and the hydrogen uptake measure directly, continuously, and in a non-invasive manner the rate of reaction, while the in situ IR spectroscopy provides time-resolved compositional information in the liq. phase. A combination of the information thus obtained leads to a clear and coherent kinetic picture of the reaction under study which can greatly



facilitate pathway anal. and mechanistic description of the catalytic reaction. In this report, the usefulness of the combination of these in situ probes is illustrated with two examples of heterogeneously-catalyzed hydrogenation reactions.

L18 ANSWER 121 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 128:175638 CA

TI Process and facility for examining chemical reactions in miniaturized **reactors** arranged parallel to each other

IN Windhab, Norbert; Miculka, Christian; Hoppe, Hans-Ulrich

PA Hoechst Research and Technology Deutschland GmbH and Co. KG, Germany

SO PCT Int. Appl., 22 pp.

PI WO 9807026 A1 19980219 WO 1997-EP4369 19970812 <--

US 6576470 B1 20030610 US 1999-242199 19991122

PRAI DE 1996-19632779 A 19960815

AB A facility and app. are described for monitoring of chem. test reactions in miniaturized **reactors** in parallel, in which the **reactors** can be analyzed with respect to the nature and degree of reaction and formation of products. The process, which involves **reactors** provided with inlet pipes and bypasses, and has **reactors** with vols. 0.001-1 cm<sup>3</sup>, is esp. useful for screening of potential catalysts and reactions under virtually identical and reproducible conditions and with a relatively low amt. of substance and samples, at low cost. The method also has application in combinatorial chem.

L18 ANSWER 126 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 128:66882 CA

TI Multicomponent surface analysis system **combined** with high pressure reaction cells for **studying** metal oxide model **catalysts**

AU Weiss, W.; Ritter, M.; Zscherpel, D.; Swoboda, M.; Schlogl, R.

CS Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin, D-14195, Germany

SO Journal of Vacuum Science & Technology, A: Vacuum, Surfaces, and Films (1998), 16(1), 21-29

AB A three chamber ultrahigh vacuum (UHV) surface anal. system combined with high pressure reaction cells has been designed. It can be used for the prepn. and **characterization** of ordered metal oxide model **catalyst** surfaces and for the **investigation** of heterogeneous **catalytic** reactions there on also under high pressures. The reaction cells are completely sepd. from the UHV anal. chambers. They can be used for oxidn. treatments and reaction studies at total pressures up to 1 bar. A new sample transfer mechanism together with sapphire sample holders and sample heating-cooling stations on the anal. chamber manipulators provides electron beam and resistive sample heating, liq. nitrogen sample cooling, and precise **thermocouple** temp. control. First exptl. results obtained on single cryst. iron oxide dehydrogenation films grown onto Pt(111) substrates are presented. These results demonstrate the capability of the system for in situ investigation of a sample surface using scanning tunneling microscopy, LEED, Auger electron spectroscopy, photoelectron emission microscopy, and temp. programmed desorption before and after catalytic reactions at high pressures.

This single crystal surface science approach provides new insight into the at. scale surface chem. of metal oxides under real catalysis conditions.

L18 ANSWER 128 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 128:53774 CA

TI An improved x-ray **reactor** chamber for the **simultaneous** structural and **catalytic characterization of catalysts**

AU Richter, K.; Doppler, P.

CS Inst. Environmental Technols., Berlin, D-12489, Germany

SO Solid State Ionics (1997), 101-103(Pt. 2), 687-695

AB The construction and the way of working of an improved X-ray **reactor** chamber (XRK) are described, designed for studies of solid state-gas reactions; a particular area of application is heterogeneous catalysis. By means of the XRK the structural and catalytic properties of Cu-SiO<sub>2</sub>, Ni-SiO<sub>2</sub>, Cu-ZnO-Al<sub>2</sub>O<sub>3</sub> and Si-Cu catalysts were investigated in situ during the stages of redn., reaction and ageing. The structure of the detected amorphous phase (Cu,Zn)-hydrotalcite was studied by the calcn. of the radial at. distribution function (RDF).

L18 ANSWER 131 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 127:335982 CA

TI Self-sustained oscillatory behavior of NO + CH<sub>4</sub> + O<sub>2</sub> reaction over titania-supported Pd catalysts

AU Ozkan, Umit S.; Kumthekar, Mahesh W.; Karakas, Gurkan

CS Department of Chemical Engineering, The Ohio State University, Columbus, OH, 43210, USA

SO Journal of Catalysis (1997), 171(1), 67-76

AB Self-sustained, regular oscillations were obsd. in NO + CH<sub>4</sub> + O<sub>2</sub> reaction over Pd/TiO<sub>2</sub> catalysts at specific temps. and O concns. This oscillatory behavior was studied **combining** NO redn. and CH<sub>4</sub> combustion reaction **studies** with addnl. **catalyst characterization** expts. performed under controlled atmospheres. The catalyst was prepd. using a wet impregnation technique with Pd-acetate as the precursor for Pd. A fixed-bed, flow **reactor** system was used to perform the NO + CH<sub>4</sub> + O<sub>2</sub> and CH<sub>4</sub> + O<sub>2</sub> reaction expts. Feed and product analyses were done online using gas chromatog.-**mass spectrometry**, chemiluminescence, and wet chem. techniques. Addnl. **catalyst characterization** was performed using thermal gravimetric anal. and high-temp., controlled-atm. X-ray diffraction techniques. Detailed anal. of oscillatory behavior indicated that oscillations in the product and reactant profiles are coupled with temp. oscillations in the catalyst. When combined with controlled-atm. characterization expts., these results, which can be reproduced in both NO + CH<sub>4</sub> + O<sub>2</sub> and CH<sub>4</sub> + O<sub>2</sub> systems, suggested the oscillations result from periodic phase changes of Pd on the surface. These cyclic phase transformations, in turn, result from temp. variations caused by varying levels of exothermicity of the 2 major reactions, namely NO redn. and CH<sub>4</sub> combustion, that are favored by metallic and oxidic sites, resp.

L18 ANSWER 135 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 127:250283 CA  
TI Oscillatory behavior of Pd/Al<sub>2</sub>O<sub>3</sub>, Pd-Pt/Al<sub>2</sub>O<sub>3</sub> and Pd/Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> in the oxidation of methane  
AU Deng, Youquan; Nevell, Thomas G.  
CS Division of Chemistry, University of Portsmouth, Portsmouth, PO1 2DT, UK  
SO Faraday Discussions (1997), Volume Date 1996, 105(Catalysis and Surface Science at High Resolution), 33-46  
AB The reaction of methane (2%) with oxygen (2.8-4.6%) in nitrogen at atm. pressure over Pd/Al<sub>2</sub>O<sub>3</sub>, Pd-Pt/Al<sub>2</sub>O<sub>3</sub> and Pd/Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> at temps. in the range 250-600°C has been **studied** using **catalytic** microcalorimeters (beads) with **simultaneous anal.** of gas mixts. by **FTIR**. With close-to-stoichiometric gas mixts., these catalysts showed oscillatory behavior at 350-550°C. Oscillations were assocd. with changes in catalytic activity due to oxidn. or redn. of the catalyst. Corresponding changes in morphol. were also implicated by the enhanced thermal emissivity of the more active partially oxidized catalyst. Oscillations were weakened over Pd/Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> but were considerably enhanced over Pd-Pt/Al<sub>2</sub>O<sub>3</sub>. Using two beads of Pd/Al<sub>2</sub>O<sub>3</sub>, interactions between oscillating systems were investigated. Heat-transfer effects were appreciable at sepns. of less than 2 mm but gas-phase communication, via changes in reactant concns., were obsd. at higher sepns. Oscillations were eliminated at very close sepns.

L18 ANSWER 163 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 125:287616 CA  
TI Combined Raman and IR study of MO<sub>x</sub>-V<sub>2</sub>O<sub>5</sub>/Al<sub>2</sub>O<sub>3</sub> (MO<sub>x</sub> = MoO<sub>3</sub>, WO<sub>3</sub>, NiO, CoO) catalysts under dehydrated conditions  
AU Vuurman, Michael A.; Stufkens, Derk J.; Oskam, Ad; Deo, Goutam; Wachs, Israel E.  
CS Dep. Chem. Eng., Univ. Amsterdam, Amsterdam, 1018WV, Neth.  
SO Journal of the Chemical Society, Faraday Transactions (1996), 92(17), 3259-3265  
AB The influence of a 2nd metal oxide (W oxide, Mo oxide, Ni oxide, Co oxide) upon a V<sub>2</sub>O<sub>5</sub>/Al<sub>2</sub>O<sub>3</sub> **catalyst** was **studied** by a **combined** Raman and **IR** study under dehydrated conditions. The presence of W or Mo oxide increases the concn. of polymd. surface V oxide species, and this reflects the higher surface coverages of the metal oxides on the alumina support. This is probably caused by competition between V and Mo oxide (for V and W oxide) species for reaction with the alumina hydroxy groups, since the IR spectra showed that on addn. of these metal oxides the same type of alumina hydroxy groups are consumed. The presence of Ni or Co oxide on alumina increases the concn. of polymd. V oxide species dramatically, which indicates that the presence of these oxides is also experienced by the surface V oxide. However, the hydroxy groups are not affected as they are for the Mo and W oxide systems.

L18 ANSWER 165 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 125:283513 CA  
TI Surface-enhanced Raman spectroscopy as an in situ real-time **probe** of

**catalytic** mechanisms at high gas pressures. The CO-NO reaction on platinum and palladium

AU Williams, Christopher T.; Tolia, Anish A.; Chan, Ho Yeung H.; Takoudis, Christos G.; Weaver, Michael J.

CS Department of Chemistry, Purdue University, West Lafayette, IN, 47907, USA

SO Journal of Catalysis (1996), 163(1), 63-76

AB Surface-enhanced Raman spectroscopy (SERS), combined with simultaneous **mass spectrometric** measurements, has been utilized to probe the reactive nature of surface species present during the redn. of NO by CO on Pt and Pd. As in our earlier studies, the SERS-active transition-metal surfaces are prepd. by electrodepositing ultrathin films onto electrochem. roughened gold. These surfaces display remarkably robust SERS activity, enabling intense Raman spectra to be obtained over a range of reactant pressures (here up to 1 atm) and at temps. up to at least 400°C. During nitric oxide adsorption at 1 atm on Pt, both terminal (240 and 470 cm<sup>-1</sup>) and bridged (325 cm<sup>-1</sup>) states of mol. NO were **detected** at lower temps. (25-200°C), with some dissocn. occurring at higher (ca 250°C) temps. as evidenced by the presence of at. nitrogen (295 cm<sup>-1</sup>). Similarly, a bridged NO species (310 cm<sup>-1</sup>) was obsd. on Pd under similar conditions, with dissocn. detected in the form of at. nitrogen (285 cm<sup>-1</sup>) and surface oxide (450 and 665 cm<sup>-1</sup>). Co-dosing of reactants on platinum produced a surface dominated by NO and CO (470 and 2080 cm<sup>-1</sup>), whereas the former was adsorbed preferentially on Pd. Simultaneous SERS/MS measurements were performed during reaction of an equimolar reactant mixt. at 1 atm of total pressure over both metals. Both CO<sub>2</sub> and N<sub>2</sub>O were formed during reaction on Pt, with onset of detectable product formation correlating with depletion of adsorbed CO and NO, resp. In contrast, CO<sub>2</sub> was the only product detected over Pd, with the depletion of surface oxygen suggesting that NO dissocn. may be rate limiting at higher temps. (ca 300°C). The extent of dissocn. on these surfaces is compared and contrasted, with particular emphasis placed on its role in detg. reaction selectivity. Furthermore, the overall behavior of these catalysts is compared with our former observations regarding this redn. process on rhodium.

L18 ANSWER 176 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 124:154297 CA

TI Fluidized bed **catalytic** combustion. **Measurement of temperature** variations in a bed

AU Takeuchi, Masao; Konno, Junko; Suzuki, Yoshizo

CS Thermal Energy and Combustion Engineering Dept., NIRE, Japan

SO Shigen to Kankyo (1995), 4(6), 429-34

LA Japanese

AB Fluidized bed catalytic combustion has excellent low NO<sub>x</sub> characteristics and high efficiency during heat utilization. Temp. variations in a bed were measured to clarify whether the life of combustion catalyst could be affected those characteristics. The fluidized material was Al<sub>2</sub>O<sub>3</sub>, in which a Pt catalyst was mixed, with a percentage wt. of 1-8. **Simultaneous** motion observations of bubbles in

the bed and **temp. measurements** of the reacting **catalyst** were conducted using a high-speed video system and an **IR** thermal camera to confirm that the max. the temp. of the catalyst itself did not exceed its crit. heat resistant temp. Results showed that temp. variations of the working catalysts were within ~30K in the exptl. conditions. Consequently, temp. variations in the bed were not affected by the life of the catalyst.

L18 ANSWER 184 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 123:303998 CA

TI A high-**temperature** Kelvin **probe** for flow reactor studies

AU Lundgren, S.; Kasemo, B.

CS Applied Physics Department, Volvo Technological Development, Goeteborg, S-412 88, Swed.

SO Review of Scientific Instruments (1995), 66(7), 3976-81

AB A vibrating capacitor device (Kelvin probe) has been developed for measurements of work-function changes  $\Delta\Phi$  during ongoing catalytic reactions up to high temps. (750 K) and atm. pressure. The construction is based on the piezoelec. actuator principle, and utilizes a lever arrangement that transfers the vibrating motion of the actuator to the ref. electrode. The lever arrangement eliminates a static load on the actuator, which therefore allows a large distance between the actuator and the vibrating ref. electrode. This makes possible much higher temp. in the reaction/sample zone than the piezoelec. actuator itself permits. The large actuator-electrode distance also reduces the risk of electromagnetic pickup in the  $\Delta\Phi$  measurements, from the driving circuit for the piezoelec. actuator. The ref. electrode is a gold disk with 3 mm diam. and a thickness of 0.1 mm. The practical  $\Delta\Phi$  resohn. is presently about 5 meV. The device has been combined with online **mass spectrometric** detection of reaction rates and its performance is illustrated by results from the H<sub>2</sub>/O<sub>2</sub> and CO/O<sub>2</sub> reactions on Pt.

L18 ANSWER 189 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 123:256100 CA

TI Structure **analysis** of highly reactive metal **catalysis** intermediates by a **combination** of **mass spectrometry** and photodetachment-ZEKE-photoelectron spectroscopy

AU Drechsler, G.; Baessmann, C.; Boesl, U.; Schlag, E. W.

CS Institut fuer Physikalische und Theoretische Chemie, Technische Universitaet Muenchen, Lichtenbergstr. 4, Garching, 85748, Germany

SO Journal of Molecular Structure (1995), 348, 337-40

AB The aim of our inquiry is a laser spectroscopic anal. and characterization of the ground state of mass selected reactive metal org. compds. A combination of neg.-ion time-of-flight **mass spectrometry** and photodetachment spectroscopy are used to study FeO and iron/acetylene systems. Two forms are used here: conventional photoelectron spectroscopy (PES), to get basic information on the system, and zero-kinetic-energy-(ZEKE-)PES, for precise measurements with a spectral resohn. down to 1.5 cm<sup>-1</sup>. Currently we are analyzing

components of the iron-acetylene system. The procedure is now being tested on ref. species: well-characterised FeO and FeC<sub>2</sub>, the smallest metal org. compd. in the iron-acetylene system. First results are shown.

L18 ANSWER 192 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 123:39877 CA

TI NO + CO reaction on Rh and CeRh-SiO<sub>2</sub> catalysts. In situ IR and temperature-programmed reaction study

AU Chuang, Steven S. C.; Krishnamurthy, Raja; Srinivas, Girish

CS Dep. Chem. Eng., Univ. Akron, Akron, OH, 44325-3906, USA

SO ACS Symposium Series (1995), 587(Reduction of Nitrogen Oxide Emissions), 183-95

AB The interaction and reaction of adsorbed NO and CO on Rh and Ce-Rh **catalysts** were **studied** by **combined** in situ IR spectroscopy and temp.-programmed reaction at 298-673 K. At 298 K, NO adsorption as NO-causes desorption of pre-adsorbed linear and bridged CO from reduced Rh sites. NO adsorption competes over CO adsorption on the reduced Rh while NO does not adsorb on oxidized Rh catalyst which chemisorbs CO as gem-dicarbonyl. The temp.-programmed reaction study revealed that the type of adsorbate and surface state of the catalyst change with temp. At 453-543 K, NO adsorbs as low wave no. NO- at 1689-1696 cm<sup>-1</sup>, which may be involved in NO dissocn., and CO adsorbs as gem-dicarbonyl which may be a spectator species for this reaction.

L18 ANSWER 196 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 122:290281 CA

TI A combined MAS nuclear magnetic resonance spectroscopy, in situ FT **infrared** spectroscopy and catalytic study of the conversion of allyl alcohol over zeolite catalysts

AU Anderson, Michael W.; Dwyer, John; Hutchings, Graham J.; Lee, Darren F.; Makarova, Marina; Zibrowius, Bodo

CS Dep. Chem., UMIST, Manchester, M60 1QD, UK

SO Catalysis Letters (1995), 31(4), 377-93

AB A **combined** study of allyl alc. conversion over zeolite **catalysts** using **catalytic measurements** in a flow **microreactor**, in situ **FTIR** and MAS NMR spectroscopy is reported. Rate consts. for the conversion in the flow **reactor** and the static in situ **reactor** used in the **FTIR** studies are in broad agreement, emphasizing the viability of the exptl. approach. In the flow **microreactor** allyl alc. conversion over the zeolite catalyst is shown to form diallyl ether, hydrocarbons and acrolein. The in situ study successfully models the formation of diallyl ether and hydrocarbon as initial reaction products, but unfortunately acrolein is found to be rapidly converted to hydrocarbons under the condition used in the in situ cells. The studies are combined to provide a model for the reaction which involves two parallel pathways for the formation of the hydrocarbons and acrolein.

L18 ANSWER 206 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 121:217120 CA

TI A new cell for in situ x-ray diffraction **studies** of **catalysts** and other

materials under reactive gas atmospheres

- AU Puxley, D. C.; Squire, G. D.; Bates, D. R.  
CS Special Techniques Group, British Gas PLC, Loughborough/Leicestershire,  
LE11 3QU, UK  
SO Journal of Applied Crystallography (1994), 27(4), 585-94  
AB A novel cell for in situ x-ray diffraction (XRD) has been designed and  
built. It allows the study of samples in flowing or static reactive  
gas environments at atm. pressure and at temps. up to 1273 K. The  
sample is supported on a quartz-glass frit between two hemispherical  
heaters. The reactant gas mixt. passes through the powder sample and  
is analyzed on exit by quadrupole **mass spectrometry** and/or gas  
chromatog. Since all the reactants pass through the sample, the  
arrangement is particularly suitable for the **study of catalysts**. This  
instrument geometry also ensures that all the diffracting sample is in  
the same environment and gives high diffracted intensity, allowing the  
system to be used with a std. x-ray source and detector. A  
**thermocouple** placed in the sample provides an accurate **measure of**  
sample **temp.**; the temp. distribution across the sample is very uniform.  
Three examples of the use of the high-temp. cell for in situ x-ray  
diffraction (XRD) are presented. These give some idea of the scope of  
expts. that can be performed in the app. Two of the examples involve  
**studies of catalysts** in various gases, the other follows the course of  
a solid-state reaction.

- L18 ANSWER 211 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 121:41769 CA  
TI Transient response of a monolithic oxidation catalyst. Effects of  
process conditions  
AU Klinghoffer, Alec A.; Rossin, Joseph A.  
CS Geo-Centers, Inc., Fort Washington, MD, 20744, USA  
SO ACS Symposium Series (1994), 552(Environmental Catalysis), 316-30  
AB The transient response of a monolithic oxidn. **catalyst** was **investigated**  
by exposing the **catalyst** to high concn. pulses of chloroacetonitrile.  
Transient response is defined as the rate at which the catalyst temp.  
(and hence activity) increases with time following a step change in  
concn. Expts. were conducted employing air inlet temps. of 365, 500,  
and 435°, challenge concns. of 5000 and 10,000 ppm (vol./vol.) and a  
residence time of 0.25 s. Both the feed and effluent concn. of  
chloroacetonitrile, and the **catalyst temp.** were **monitored**  
**simultaneously** in real time. The results indicate that increasing the  
challenge concn. from 5000 to 10,000 ppm (vol./vol.) greatly increases  
the transient response of the catalyst. Also, for air inlet temps. of  
435°, the rapid increase in the catalyst temp. results in >99.9%  
removal of the challenge dose.

- L18 ANSWER 214 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 120:254629 CA  
TI A **combined** QEXAFS/XRD method for online, in situ **studies of catalysts**:  
examples of dynamic **measurements** of copper-based methanol catalysts  
AU Clausen, Bjerne S.; Graabaek, Lars; Steffensen, Gert; Hansen, Poul L.;  
Topsoe, Henrik

CS Haldor Topsoe Res. Lab., Lyngby, DK-2800, Den.  
SO Catalysis Letters (1993), 20(1-2), 23-36  
AB The development of a new in situ method which allows high quality XRD and EXAFS to be obtained online under ideal catalytic conditions is discussed. The possibility to obtain both types of information simultaneously enables a much better structural description of catalytic materials which typically contain both cryst. and x-ray amorphous structures. The system employs a capillary tube as the **microreactor**/in situ cell. The high degree of temp. uniformity of the cell and the possibilities of fast changes in reaction conditions make the system ideal for dynamic studies. For this purpose, the EXAFS measurements are carried out in the newly developed quick scanning mode (QEXAFS) which also allows high quality data to be obtained. The XRD is acquired using a position sensitive detector. The application of the setup for time resolved measurements is demonstrated in a study of the calcination and redn. of Cu-based methanol catalysts where the changes take place over a few degrees. The high quality of the data made it possible to obtain important new insight regarding the presence of intermediate phases during these processes. Studies of Cu/SiO<sub>2</sub> catalysts show the advantages of a newly developed theory for a better estn. of coordination nos. (and thus particle sizes) from EXAFS.

L18 ANSWER 229 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 118:246372 CA

TI A new attachment for non-ambient x-ray powder diffraction studies in various atmospheres

AU Richter, K.; Peplinski, B.; Doppler, P.

CS Anal. Cent. Berlin-Adlershof, Berlin, O-1199, Germany

SO Materials Science Forum (1991), 79-82 (EPDIC 1, Pt. 1), 439-44

AB A new combination of anal. instruments was realized, consisting of a sophisticated x-ray heating chamber in connection with com. instruments (x-ray powder diffraction goniometer, gas chromatographs, temp. controller, gas supply system with electronic mass flow controller). It allows to pretreat and to run catalysts in oxidizing, inert, and reducing atmospheres at temps. up to 500° at hourly space velocities up to 10,000 v/vh and to carry out **simultaneously** a comprehensive structural **characterization** of the **catalysts** by a wide variety of x-ray diffraction techniques and to analyze permanently the compn. of the gas flow passing through the catalyst sample. The design of the x-ray **reactor** chamber is described. The chamber has been used for the investigation of the kinetics, of the active state, and of the aging of Cu-ZnO-Al<sub>2</sub>O<sub>3</sub> catalysts, active in the methanol synthesis.

L18 ANSWER 238 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 117:220909 CA

TI Interactions of sulfur dioxide with palladium, cerium, palladium-chromium, and Pd-Ce catalysts on  $\gamma$ -alumina supports

AU Umbetkaliev, A. K.; Dosumov, K.; Popova, N. M.

CS Inst. Org. Katal. Elektrokhim. im. Sokol'skogo, Almatz, Kazakhstan

SO Zhurnal Fizicheskoi Khimii (1992), 66(8), 2229-31

LA Russian



AB The interactions of SO<sub>2</sub> with Pd-, Ce-, Cr-, Pd-Cr-, and Pd-Ce- $\gamma$ -Al<sub>2</sub>O<sub>3</sub> **catalysts** at various temps. were **studied** by temp.-programmed redn. **combined** with **mass spectrometry** and gas chromatog. The nature of the interaction varies with the nature of the metals; the amts. of SO<sub>2</sub> desorbing (an inverse measure of the degree of sulfation or poisoning) decrease in the order Al<sub>2</sub>O<sub>3</sub> > Pd-Ce-Al<sub>2</sub>O<sub>3</sub> > Ce-Al<sub>2</sub>O<sub>3</sub> > Pd-Al<sub>2</sub>O<sub>3</sub> > Cr-Al<sub>2</sub>O<sub>3</sub> > Pd-Cr-Al<sub>2</sub>O<sub>3</sub>. Activation energies of SO<sub>2</sub> desorption range from 37.7 to 121.3 kJ mol<sup>-1</sup>.

L18 ANSWER 253 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 115:264315 CA

TI In situ cell for **combined** XRD and on-line **catalysis tests: studies** of copper-based water gas shift and methanol catalysts

AU Clausen, B. S.; Steffensen, G.; Fabius, B.; Villadsen, J.; Feidenhans'l, R.; Topsoe, H.

CS Haldor Topsoe Res. Lab., Lyngby, DK-2800, Den.

SO Journal of Catalysis (1991), 132(2), 524-35

AB A newly developed in situ x-ray diffraction (XRD) cell was used to obtain information on the structure of binary Cu-Zn and ternary Cu-Zn-Al catalysts during redn. and water gas shift and MeOH synthesis. A major advantage of the cell is that it also serves as an ideal plug flow catalytic **reactor** such that realistic catalytic and structural information can be obtained simultaneously on the same sample. The cell can be operated both at high temps. and high pressures. Direct MeOH activity tests confirmed the suitability of the cell. By use of x-rays from a synchrotron source, dynamic studies on the time scale of seconds are demonstrated. This feature was used to study the phase transformation occurring during the activation of the calcined catalysts. In the active catalysts, Cu metal is the only cryst. Cu phase observed, and the formation of this phase is closely related to the disappearance of CuO in the calcined catalyst. The XRD results provide detailed information on the nucleation and growth processes. The variation in the water gas shift activity correlates with the changes in the Cu surface area.

L18 ANSWER 254 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 115:216137 CA

TI Methods and apparatus for the **simultaneous** execution of roentgenographic and **catalytic investigations** of reactive powders

IN Richter, Klaus; Peplinski, Burkhard; Steinert, Gerhard

PA Akademie der Wissenschaften der DDR, Germany

SO Ger. (East), 7 pp.

PI DD 286872 A5 19910207 DD 1989-331697 19890811 <--

PRAI DD 1989-331697 19890811

AB The title methods entail exposing a sample of the powder of interest to x radiation while heating and directing a gas stream through it so that, while the diffracted x-rays are recorded, the chem. compn. of the gases is continuously monitored and the instantaneous catalytic activity of the sample is detd. App., incorporating an x-ray diffractometer, a gas introduction system, a gas anal. system, and an electronic temp. regulation system, for carrying out the methods is

also described.

- L18 ANSWER 263 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 114:254669 CA  
TI **Combined** in-situ **FTIR** and on-line activity **studies**: applications to vanadia-titania DeNOx **catalyst**  
AU Topsoe, Nan Yu; Topsoe, Henrik  
CS Haldor Topsoe Res. Lab., Lyngby, DK-2800, Den.  
SO Catalysis Today (1991), 9(1-2), 77-82  
AB An approach for performing combined in-situ **FTIR** and online activity measurements is described. The application of such studies to V2O5-TiO2 DeNOx catalysts is given. The trends in catalytic activity measured directly with the **FTIR** cell/**reactor** agreed with sep. activity measurements demonstrating that the present exptl. approach provides a direct link between the surface chem. and the catalysis. During the DeNOx reaction conditions, both Broensted and Lewis acid sites are present on the surface and they adsorbed NH3 strongly. The surface V-OH and V = O groups are probably involved in the catalytic reaction.
- L18 ANSWER 285 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 109:237987 CA  
TI In situ EXAFS studies of small iron particles used as catalysts for ammonia synthesis  
AU Niemann, W.; Clausen, B. S.; Topsoe, H.  
CS Haldor Topsoe Res. Lab., Lyngby, DK-2800, Den.  
SO NATO ASI Series, Series B: Physics (1987), 158(Phys. Chem. Small Clusters), 909-14  
AB Supported Fe particles used as **catalysts** for NH3 synthesis were **studied** by x-ray absorption measurements under real reaction conditions. Starting with the precursor, various redn. stages and the final reaction conditions at high pressure and high temp. (80 bar, 400°) were investigated. The redn. of Fe oxide and the growth of Fe particles was directly obsd. in EXAFS. **Simultaneously**, the activity of the **catalyst** was **measured**. A comparison with the EXAFS of an Fe foil **measured** at the same **temp.** gives indications of the size of the small Fe particles in the catalyst.
- L18 ANSWER 288 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 109:135781 CA  
TI **Study** of model copper-based **catalysts** by **simultaneous** differential scanning calorimetry, x-ray diffraction and **mass spectrometry**  
AU Newman, Robert A.; Blazy, Joseph A.; Fawcett, Timothy G.; Whiting, Larry F.; Stowe, Robert A.  
CS Michigan Applied Sci. Technol. Lab., Dow Chem. USA, Midland, MI, 48667, USA  
SO Materials Research Society Symposium Proceedings (1988), 111(Microstruct. Prop. Catal.), 405-11  
AB The results of this study show Cu2O as an intermediate in the redn. of the CuO portion of each of the model catalysts. Such features as the onset temp. and Cu surface area varied widely among the 4 catalysts in response to the same chem. event conducted under similar exptl.

conditions. Oxidn. runs on the reduced catalysts were all similar, 1 producing Cu<sub>2</sub>O from metal over a broad range of temp., followed by the oxidn. of CuO at even higher temps.

L18 ANSWER 298 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 108:211046 CA

TI Temperature-programmed desorption and **infrared** study of carbon monoxide and hydrogen adsorption on copper/zinc oxide catalysts

AU Roberts, D. L.; Griffin, G. L.

CS Dep. Chem. Eng. Mater. Sci., Univ. Minnesota, Minneapolis, MN, 55455, USA

SO Journal of Catalysis (1988), 110(1), 117-26

AB A series of Cu/ZnO **catalysts** prepd. by several methods were **characterized** by using a **combination** of adsorbate uptake **measurements**, **temp.**-programmed desorption, and Fourier transform IR spectroscopy applied to CO, H<sub>2</sub>, and O<sub>2</sub> adsorbates. Adsorbed CO is present on the reduced catalysts in several adsorption states, which desorb with apparent activation energies of 10-16 kcal/mol. When CO is adsorbed on oxidized catalysts, the frequencies shift to higher energy and the highest desorption energy increases to 19 kcal/mol. For H<sub>2</sub> adsorbed on reduced catalysts, a single desorption state which has an apparent activation energy of 20-21 kcal/mol is obsd. When H<sub>2</sub> is adsorbed on oxidized catalysts, the desorption energy of this state increases to 26-27 kcal/mol. For the reduced catalysts, the amts. of reversible CO and H<sub>2</sub> adsorbed correlate linearly with the amt. of O<sub>2</sub> chemisorption measured at 98 K, with relative uptakes for CO, H<sub>2</sub>, and O<sub>2</sub> in the ratio 9:2:10. These results are interpreted as Cu being present as metallic clusters which expose a large fraction of high-index surface planes. The chem. behavior of these planes is significantly different from that of low-index single crystal planes.

L18 ANSWER 302 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 108:74787 CA

TI **Simultaneous** differential thermal analysis and **mass spectrometry** for the **study** of **catalytic** reactions

AU Rogers, Donald Evan

CS DSIR, Petone, N. Z.

SO Sciencaj Komunikajoj (1986), 11, 44-52

LA Esperanto

AB A DTA sample holder was modified to allow a reactant-contg. gas to flow through a small catalyst bed and then via a heated line to a quadrupole **mass spectrometer**. The speed of the anal. permitted const. or pulsed operation. MeOH dehydration over HZSM-5 zeolite showed relations between adsorption, desorption, heat of reaction, and product compn. as functions of time and temp.

L18 ANSWER 306 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 107:142196 CA

TI Integrated kinetic modeling and transient **FTIR** studies of carbon monoxide oxidation on platinum/silica

AU Kaul, D. J.; Sant, R.; Wolf, E. E.

CS Chem. Eng. Dep., Univ. Notre Dame, Notre Dame, IN, 46556, USA  
SO Chemical Engineering Science (1987), 42(6), 1399-411  
AB The reaction dynamics and multiplicity features of CO oxidn. on a Pt/SiO<sub>2</sub> **catalyst** are **studied** via transient expts. **combining** Fourier transform IR spectroscopy (**FTIR**) with temp.-programmed reaction (TPR) and with concn.-programmed reaction (CPR). Bifurcation diagrams of the surface and bulk concns. and temps. obtained in these expts. are used to develop a reaction-**reactor** model. The model integrates non-equil. elementary step kinetics, based on single-crystal studies, with heat and mass transport effects and **reactor** modeling. The model reproduces bifurcation cross-section diagrams at various exptl. conditions and simulates the TPR and CPR expts. A parametric sensitivity anal. reveals how changes in the parameters affect the reaction behavior, as well as how the rate-detg. step changes with the operating conditions. The results demonstrate how the many interactions between the kinetics, transport processes, and **reactor** environment affect exptl. observations, and provide a method for the proper assessment of such interactions.

L18 ANSWER 311 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 106:220868 CA  
TI Dissociation reactions of carbon monoxide gas on iron and iron oxide (Fe<sub>2</sub>O<sub>3</sub>) surfaces observed by Raman-ellipsometry spectroscopy  
AU Watanabe, Masao; Kadowaki, Toru  
CS Res. Inst. Catal., Hokkaido Univ., Sapporo, 060, Japan  
SO Applied Surface Science (1987), 28(2), 147-66  
AB A **combined** system of Raman spectroscopy and ellipsometry was developed for the **study** of **catalyst** surfaces on which a chem. reaction is taking place. The dielec. function and the thickness of a surface layer or a surface compd. produced in the reaction are analyzed by ellipsometry; vibrational modes of the compd. and surface species are analyzed by Raman spectroscopy, and the products in the gas phase by **mass spectrometry**. The system was applied to the study of the Boudouard and dissocn. reactions of CO mols. in Fe and Fe<sub>3</sub>O<sub>4</sub> catalysts. A surface layer produced by diffused C and O atoms, a thin oxide layer produced on Fe by CO dissocn., and graphite layers produced by the Coudouard reaction were analyzed. Raman spectra reveal the existence of several kinds of C species, such as defective graphite and an Fe carbide formed on the Fe and Fe<sub>3</sub>O<sub>4</sub> surfaces. Several Raman bands may be due to microscopic clusters of surface graphite. The reaction of the defective graphite with H<sub>2</sub> gas is stepwise on a time scale of seconds.

L18 ANSWER 322 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 105:140595 CA  
TI On the mechanism of the catalytic reaction of hydrogen sulfide with sulfur dioxide over γ-alumina  
AU Karge, Hellmut G.; Dalla Lana, Ivo G.; Terevizan de Suarez, Silvia; Zhang, Yingzhen  
CS Fritz-Haber-Inst., Max-Planck-Ges., Berlin, Fed. Rep. Ger.  
SO Int. Congr. Catal., [Proc.], 8th (1985), Meeting Date 1984, Volume 3, III 453-III 463 Publisher: Verlag Chemie, Weinheim, Fed. Rep. Ger.

AB SO<sub>2</sub> adsorption and interaction with H<sub>2</sub>S on an Al<sub>2</sub>O<sub>3</sub> Claus **catalyst** was **investigated** by **IR**, **combined IR/ESR**, volumetric adsorption measurements, **combined IR/GC** conversion measurements, and TPD. SO<sub>2</sub> chemisorbed on basic sites was detd. by an **IR** low-frequency band (LFB) at ~1070 cm<sup>-1</sup>. TPD studies confirm comparable amts. of irreversibly adsorbed SO<sub>2</sub> at ≤825 K. The LFB species was detected by **IR** on the surface of the working catalyst and was reactive towards H<sub>2</sub>S in a dynamic manner. There was a 2nd coexisting surface species, SO<sub>2</sub><sup>-</sup>, which was unrelated to the LFB species in both desorption trends and adsorbed amts. (only 0.1-1% of the total LFB chemisorbate). Dissocn. of SO<sub>2</sub> proceeded by exchange of O with lattice O on the Al<sub>2</sub>O<sub>3</sub> surface. The H of the surface OH groups was mobile. These results provide a somewhat improved view of steps relevant to the Claus reaction mechanism.

L18 ANSWER 327 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 105:12873 CA

TI Apparatus for **combined studies** of heterogeneously **catalyzed** reactions in the normal pressure range and surface-specific **analysis** of the **catalysts** used in the ultrahigh vacuum range

AU Borgmann, Dieter; Strattner, Peter; Wedler, Gerd

CS Inst. Phys. Theor. Chem., Univ. Erlangen-Nuernberg, Erlangen, 8520, Fed. Rep. Ger.

SO Chemie Ingenieur Technik (1986), 58(5), 400-2

LA German

AB An app. is described. It is used for normal pressure and UH V studies of heterogeneous reactions and is equipped with a **mass spectrometer** and AES spectrometer for **catalyst** surface **studies**.

L18 ANSWER 346 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 100:164521 CA

TI A new cell for **combined IR** and ESR **investigations** on solid **catalysts**

AU Karge, H. G.; Trevizan de Suarez, S.; Dalla Lana, I. G.

CS Fritz-Haber-Inst., Max-Planck-Ges., Berlin, D-1000/33, Fed. Rep. Ger.

SO Journal of Physical Chemistry (1984), 88(9), 1782-4

AB Design and operation of a new cell for **combined ESR** and **IR measurements** on **catalyst** samples such as oxides, zeolites, and supported metal particles is described. As an example, the cell is used for studies of SO<sub>2</sub> adsorption on Al<sub>2</sub>O<sub>3</sub>. ESR and **IR** investigations on one and the same Al<sub>2</sub>O<sub>3</sub>/SO<sub>2</sub> sample, showed that a low-frequency band of chemisorbed SO<sub>2</sub> is due to neutral surface species rather than SO<sub>2</sub>-radicals.

L18 ANSWER 348 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 100:109792 CA

TI **Reactor** for **combined** surface spectroscopic analysis and atmospheric pressure kinetic **studies** of **catalysts**

AU Weimer, Jeffrey J.; Putnam, Fredrick A.

CS Cent. Mater. Sci. Eng., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA

SO Review of Scientific Instruments (1984), 55(2), 238-43

AB A novel **reactor** system is described which permits ultrahigh-vacuum

surface spectroscopic studies and atm. pressure reactions to be done without a dedicated app. This system can be applied to studies of metal single crystals, although its use for kinetic studies of such samples is limited in the present design. The **reactor** was used to study the surface properties and reaction characteristics of Pt deposited on a sapphire surface. The major use of the system is to study such model-supported catalysts without exposing the sample to atm. contamination.

L18 ANSWER 352 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 99:164674 CA

TI A **combined** instrument for the **investigation** of **catalytic** reactions by means of gas chromatography, secondary ion and gas phase **mass spectrometry**, Auger and photoelectron spectroscopy, and ion scattering spectroscopy

AU Ganschow, O.; Jede, R.; An, L. D.; Manske, E.; Neelsen, J.; Wiedmann, L.; Benninghoven, A.

CS Phys. Inst., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.

SO Journal of Vacuum Science & Technology, A: Vacuum, Surfaces, and Films (1983), 1(3), 1491-506

AB A **combined** instrument was developed which couples a **microreactor** operated with tech. **catalysts** with a **combined** surface anal. instrument. The **microreactor** is equipped with gas chromatog. and gas-phase **mass spectrometry** for continuous control of the reaction parameters. The surface anal. part of the instrument incorporates secondary ion and thermal desorption **mass spectrometry**, Auger and photoelectron spectroscopy, and ion backscattering spectroscopy, all of which were developed to their full versatility and efficiency. The transfer of the catalyst from the **reactor** to the surface anal. station is performed by a valveless lock within ~1 min in a vacuum free of org. contaminations. The whole system can be operated fully under computer control. First applications of this instrument were devoted to the oxidn. of MeOH to H<sub>2</sub>CO on Ag catalysts.

L18 ANSWER 356 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 98:201322 CA

TI Hydrocarbon production by catalytic cracking of palm oil by-products

AU Graille, J.; Geneste, P.

CS Dep. Chim. Corps Gras, IRHO GERDAT, Montpellier, 34032, Fr.

SO Comm. Eur. Communities, [Rep.] EUR (1983), EUR 8245, Energy Biomass, 830-5

LA French

AB The available biomass from palm oil mills and its energy balance are presented. The solid fraction can be used to produce gasoline by cracking. A cracking **reactor** was devised allowing a **complete** control of the reaction and for **testing** several **catalysts**. The octane no. of the crude liq. effluent is 60-70. Depending on the catalyst, it is possible to produce gasoline, diesel fuel, arom. hydrocarbons for industrial org. synthesis, and a suitable solvent for the recovery of residual oil from the fibrous press cake. The energy for the process is supplied by the combustion of the byproducts.

L18 ANSWER 364 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 97:45112 CA  
TI A **combined infrared** and gas chromatographic reaction system for in situ **catalytic studies**  
AU Miura, Hiroshi; Gonzalez, Richard D.  
CS Dep. Chem., Univ. Rhode Island, Kingston, RI, 02881, USA  
SO Journal of Physics E: Scientific Instruments (1982), 15(3), 373-7  
AB A novel flow system including an **IR** cell with the capability of operating either as a pulse **microreactor** or a single-pass differential flow **reactor** was constructed. With this new design, extensive in situ surface characterization studies of working catalysts can be made. The following applications are considered: temp. programed reaction and desorption studies; the measurement of extinction coeffs., turnover nos. and activation energies, product distribution, and the surface coverage of adsorbed species under reaction condition. As an example, the reaction  $\text{CO(g)} + \text{H}_2\text{(g)}$  on  $\text{SiO}_2$ -supported Pt-Ru bimetallic clusters is considered. Results obtained using the **IR** cell as a single-pass **reactor** agree well with those obtained using a powd. catalyst placed in a conventional **microreactor**.

L18 ANSWER 383 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 92:85759 CA  
TI A design for a combined **infrared** cell/differential single-pass **reactor**  
AU Vannice, M. A.; Moon, S. H.; Twu, C. C.; Wang, S. Y.  
CS Dep. Chem. Eng., Pennsylvania State Univ., University Park, PA, 16802, USA  
SO Journal of Physics E: Scientific Instruments (1979), 12(9), 849-52  
AB An **IR** cell which also acts as a differential plug-flow **reactor** is described. The cell allows **IR** spectra and catalytic activities to be obtained simultaneously under defined reaction conditions. In addn., the cell enables prepn. of catalyst wafers which act as differential catalyst beds. The cell is durable and constructed from com. available parts.

L18 ANSWER 388 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 90:89763 CA  
TI On stream computer controlled gas chromatograph for the **analysis** of interreactor **catalytic** reformer products  
AU Stockinger, J. H.; Callen, R. B.; Kaufman, W. E.  
CS Res. Dep., Mobil Res. Dev. Corp., Paulsboro, NJ, USA  
SO Journal of Chromatographic Science (1978), 16(9), 418-26  
AB An on-stream gas-chromatog. system was developed to **evaluate** the performance of exptl. reforming **catalysts**. The system analyzes a total **reactor** vapor-phase sample obtained as the effluent from any one of the multiple **reactors** of the reformer chain. This interreactor sampling capacity permits multiple space-velocity and severity data to be obtained from one equilibrated run condition. Evaluation of reformer processes which use several types of catalyst in a cascading **reactor** configuration is also possible. The chromatog. system consists of 4 high-resoln. columns in 2 temp. zones and 2 flame ionization detectors.

Temp. and flow programming are used to optimize peak resolu. Up to 280 components were identified in certain wide-boiling-range products. Product properties such as octane no., sp. gr., mol. wt., and vapor pressure can be calcd. from the interreactor anal. Interreactor effluent compns. and calcd. properties agree with those obtained by std. mass balance methods. The vapor-phase sampling system, and other functions assocd. with gas chromatog., are controlled by a minicomputer.

- L18 ANSWER 392 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 88:95468 CA  
TI A rapid method for **catalyst** activity **measurements** by **combination** of pulse **reactor**, **mass spectrometer** and process computer  
AU Latzel, J.  
CS Inst. Phys. Chem., Tech. Univ., Vienna, Austria  
SO Reaction Kinetics and Catalysis Letters (1977), 7(4), 393-6  
AB The combination of a pulse **reactor** attached directly (without a sepn. column) to a **mass spectrometer**-process computer system is described. In order to obtain a conversion-temp. diagram for the dehydration and dehydrogenation of 2-butanol <1 h is required. Therefore, the method can be used for rapid characterization or comparison of the activities of various samples.
- L18 ANSWER 393 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 87:190033 CA  
TI Flow **reactor** for kinetic studies with **simultaneous** x-ray phase **analysis** of a **catalyst**  
AU Borodzinski, A.; Janko, A.  
CS Inst. Phys. Chem., Pol. Acad. Sci., Warsaw, Pol.  
SO Reaction Kinetics and Catalysis Letters (1977), 7(2), 163-9  
AB A flow **reactor** for kinetic **studies** of heterogeneous **catalytic** reactions with **simultaneous** x-ray phase **anal.** of the **catalyst** is described. As an example, the correlation between the selectivity of acetylene hydrogenation and the  $\beta$ -Pd hydride concn. in Pd catalysts is shown.
- L18 ANSWER 402 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 84:185418 CA  
TI Study of the formation and reactivity of surface isocyanate on palladium/aluminum oxide catalysts  
AU Solymosi, F.; Sarkany, J.  
CS Gas Kinet. Res. Group, Hung. Acad. Sci., Szeged, Hung.  
SO Reaction Kinetics and Catalysis Letters (1975), 3(3), 297-9  
AB The formation and reactivity of an isocyanate complex on a Pd/Al<sub>2</sub>O<sub>3</sub> **catalyst** was **investigated** by adsorption **measurements** and by **ir** spectroscopy **combined** with **mass spectrometry**. Adsorption studies indicate that the uptake of gases during the coadsorption of NO + CO is significantly larger than the sum of the separately adsorbed gases. The reactivity of surface isocyanate towards H<sub>2</sub>O, H<sub>2</sub>, NO, and O<sub>2</sub> was studied. The reactivity order at 200° is H<sub>2</sub>O » O<sub>2</sub> > H<sub>2</sub> > NO. **Mass spectrometric** anal. revealed the formation of NH<sub>3</sub> in the surface reaction between -NCO and H<sub>2</sub>O.



L18 ANSWER 411 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 81:62858 CA  
TI Development of a gas chromatograph-mass spectrometer with on-line computer for **studies** in **catalysis**. Reactions of ethylene and deuterium on oxides  
AU Kemball, C.; Nisbet, J. D.; Robertson, P. J.; Scurrall, M. S.  
CS Dep. Chem., Univ. Edinburgh, Edinburgh, UK  
SO Proceedings of the Royal Society of London, Series A: Mathematical, Physical and Engineering Sciences (1974), 338(1614), 299-310  
AB An on-line computer is used in a **combined** gas chromatog.-**mass spectroscopy** technique for the **study** of heterogeneous **catalysis** in the reactions of C<sub>2</sub>H<sub>4</sub> and D on oxides. The selectivities shown by the catalysts for the exchange and addn. reactions is discussed. MgO effects the exchange of C<sub>2</sub>H<sub>4</sub> without production of C<sub>2</sub>H<sub>6</sub> even at 671°K; γ-Al<sub>2</sub>O<sub>3</sub> also exhibits a high selectivity for exchange. In contrast, on Cr<sub>2</sub>O<sub>3</sub> at 197°K and ZnO at 273°K, C<sub>2</sub>H<sub>4</sub> undergoes rapid deuteration without exchange of the olefin. For the range of **catalysts studied** the ratio of rate consts. for the exchange and addn. reactions decreases in the order: MgO > Al<sub>2</sub>O<sub>3</sub> » TiO<sub>2</sub> ~ Fe<sub>2</sub>O<sub>3</sub> > Co<sub>3</sub>O<sub>4</sub> > ZrO<sub>2</sub> » ZnO ~ Cr<sub>2</sub>O<sub>3</sub>. The differences in catalytic behavior of the oxides is also discussed.

L18 ANSWER 412 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 81:30199 CA  
TI Batch **reactor** to study concomitant adsorption and heterogeneous catalysis  
AU Hsu, Stephen M.; Kabel, Robert L.  
CS Dep. Chem. Eng., Pennsylvania State Univ., University Park, PA, USA  
SO Journal of Catalysis (1974), 33(1), 74-82  
AB A batch **reactor** has been devised in which adsorption phenomena important to a heterogeneous catalytic reaction can be followed simultaneously with the overall reaction process. The experimental technique is illustrated with the vapor phase dehydration of EtOH to Et<sub>2</sub>O as catalyzed by H exchange resin. Directly measured data are vapor phase composition, total adsorption, and total pressure as functions of time. Derived results are adsorbed phase composition data, fractional conversion, the thermodynamic equilibrium constant, and an independent check on internal consistency. The method inherently provides insights characteristic of dynamic experiments while retaining the simplicity of a set of 1st-order ordinary differential equations for any mathematical treatment desired. For this catalytic reaction the adsorption processes are shown, without recourse to theor. analysis, to be much faster than the surface reaction.

L18 ANSWER 419 OF 471 CA COPYRIGHT 2004 ACS on STN  
AN 77:144315 CA  
TI Automated **reactor** system for catalyst research  
AU Hogan, R. J.; Doane, E. P.  
CS Res. Dev. Dep., Phillips Pet. Co., Bartlesville, OK, USA  
SO Preprints - American Chemical Society, Division of Petroleum Chemistry

(1971), 16(2), D35-D42

AB A **fully** automatic **microreactor** unit for **catalytic studies** is described. The system provides the means for obtaining data on catalytic reactions quickly, accurately, and with a min. amt. of attention. It can be adapted easily to a variety of expts., including reaction kinetics, catalyst screening, and process variable studies. The unit employs a central master programmer to conduct unattended expts. with 6 **reactors**, and a high speed analyzer-integrator system to collect and analyze samples on command, and record the results on paper tape.

L18 ANSWER 428 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 72:91942 CA

TI Characterization of gas oil stocks: an integrated analysis

AU Fitzgerald, Maurice E.; Moirano, J. L.; Morgan, Harry; Cirillo, V. A.

CS Arco Chem. Co. Div., Atl. Richfield, Philadelphia, PA, USA

SO Applied Spectroscopy (1970), 24(1), 106-14

AB Gas oil stocks (virgin, **catalytically** cracked, or blended) are **characterized** by a **combination** of anal. techniques. A hydrocarbon type anal. of the sats., normal and isoparaffins, and of cycloparaffins and aromatics by detailed ring structure permits correlation of feed compns. with coke-producing properties and product distributions for catalytic cracking. A polynuclear aromatic uv anal. is obtained from the total sample; another portion is sepd. into sat. and aromatic fractions by a liq. chromatog. **Mass spectrometer** anal. on each fraction coupled with the uv anal. and a mol. sieve sepn. on the sat. fraction for % normal paraffins allow a complete hydrocarbon-type distribution. In the case of catalytically cracked stocks, S compds. contribute to the uv spectrum; to correct the uv, S detn. is necessary. Wt. % polynuclear aromatics are obtained solely from the uv with the aid of b.p. and mol. wt. correlations.

L18 ANSWER 444 OF 471 CA COPYRIGHT 2004 ACS on STN

AN 67:26065 CA

TI New **test** apparatus for **catalysts**

AU Guyer, A., Jr.

CS Tech. Chem. Lab. ETH, Zurich, Switz.

SO Chimia (1967), 21(3), 134-5

LA German

AB A new app. for **testing** single **catalyst** grains in continuous or pulsed streams, **combined** with grain **temp. measurement** and gas chromatographic analysis is described.

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